### PROGRAM

Sunday, November 22, 2015				
9:00-9:10		Opening Remarks by Koichi Kato		
		Chair : Hisashi Okumura		
9:10-9:50	L01	Tigran Chalikian (University of Toronto)		
		"Volumetric insights into protein-cosolvent interactions"		
9:50-10:20	L02	Ryo Akiyama (Kyushu University)		
		"Effective attraction between negatively charged sites on proteins and ordering of		
		proteins in an electrolyte solution"		
10:20-10:50		Coffee Break		
		Chair : Tomohisa Sawada		
10:50-11:30	L03	Michaele J. Hardie (University of Leeds)		
		"Self-assembly, ligand exchange and chiral self-sorting of coordination cages"		
11:30-12:00	L04	Kazuyoshi Murata (National Institute for Physiological Sciences)		
		"Dynamical ordering of virus particle for creation of integrated functions"		
12:00-12:40		Poster preview (only poster prize candidates)		
12:40-13:00		Group photo		
13:00-14:30		Lunch		
14:30-16:30		Poster Session 1 (Odd Poster Number)		
		Chair : Eri Chatani		
16:30-17:10	L05	Pau Bernadó (Centre de Biochimie Structurale)		
		"A structural perspective of biological function and malfunction of intrinsically disordered proteins"		
17:10-18:10		Panel discussion		
18:20-		Banquet		

### Monday, November 23, 2015

		Chair : Yukiko Kamiya
9:10-9:50	L06	David Wales (University of Cambridge)
		"Energy landscapes: ordering and function"
9:50-10:20	L07	Kazunori Sugiyasu (National Institute for Materials Science)
		"Dynamic ordering of supramolecular assemblies developed on a complex energy
		landscape"
10:20-10:50		Coffee Break
		Chair : Ken Sato
10:50-11:30	L08	Thomas Surrey (The Francis Crick Institute)
		"Systems biochemistry of the microtubule cytoskeleton: mechanistic insight from
		reverse engineering"
11:30-12:00	L09	Kensaku Mizuno (Tohoku University)
		"Dynamic reordering of actin cytoskeleton in mechanical force-induced cell
		responses"
12:00-12:30	L10	Tomoaki Matsuura (Osaka University)
		"Dynamics of biological systems constructed in vitro"
12:30-14:00		Lunch
14.00.16.00		
14:00-16:00		Poster Session 2 (Even Poster Number)
16:00		Closing Remarks by Koichi Kato

### **Poster sessions**

### Date

Poster session 1: 14:30-16:30, Sunday, November 22 Odd Poster Numbers (P001, P003, P005 ... P093)

Poster session 2: 14:00-16:00, Monday, November 23 Even Poster Numbers (P002, P004, P006 ... P094)

- All posters should be put on the boards by 14:30 on Sunday, November 22, and be removed between 16:00 and 16:30 on Monday, November 23
- Presenting authors are requested to stay with their posters during the session time above.

### Banquet

### Date

18:20-, Sunday, November 22

### Place

Nishijin Plaza 1F Hall

### List of Posters

### P001 Structural insights into intracellular quality control of glycoproteins mediated by their glucosylation

<u>Tong Zhu</u><sup>1,2,3</sup>, Tadashi Satoh<sup>3</sup>, Takumi Yamaguchi<sup>1,2,3</sup>, and Koichi Kato<sup>1,2,3</sup> <sup>1</sup>School of Physical Sciences, SOKENDAI, <sup>2</sup>Institute for Molecular Science and Okazaki Institute for Integrative Bioscience, National Institutes of Natural Sciences, <sup>3</sup>Graduate School of Pharmaceutical Sciences, Nagoya City University

### P002 Exploration of micro-macro relationships in dynamic ordering of biomolecular systems and their underlying design principles

<u>Koichi Kato</u><sup>1,2</sup>, Tadashi Satoh<sup>2</sup>, Takumi Yamaguchi<sup>1,2</sup>, and Maho Yagi-Utsumi<sup>1,2</sup> <sup>1</sup>Okazaki Institute for Integrative Bioscience, National Institutes of Natural Sciences, <sup>2</sup>Graduate School of Pharmaceutical Sciences, Nagoya City University

P003 Three-dimensional protein structure and dynamics in living cells
 <u>Teppei Ikeya<sup>1</sup></u>, Jin Inoue1, Peter Güntert<sup>1,2</sup> and Yutaka Ito<sup>1</sup>
 <sup>1</sup>Graduate School of Science and Engineering, Tokyo Metropolitan University
 <sup>2</sup>Institute of Biophysical Chemistry, Goethe University Frankfurt, Germany

### P004 Ultimate sensitive laser microscopy for biomolecules dissolved in a trapped microdroplet Kenji Sakota, Hiroshi Sekiya Department of Chemistry, Kyushu University

- P005 Single-molecule imaging of GPCR oligomerization followed by internalization
   Masataka Yanagawa, Micho Hiroshima, and <u>Yasushi Sako</u>
   Cellular Informatics Laboratory, RIKEN
- P006 Creation of ATP-driven cyborg rotary molecular motors
   <u>Ryota Iino</u><sup>1,2</sup>
   <sup>1</sup>Okazaki Institute for Integrative Bioscience, <sup>2</sup>Institute for Molecular Science
- P007 Influence of the secondary structure of proteins on its rotational diffusion coefficients <u>Tomoyuki Yoshitake</u>, Masahide Terazima Graduate School of Science, Kyoto University

#### P008 Site-specifically fluorescent-labeled proteins for sensing and controlling protein functions

<u>Takahiro Hohsaka</u>, Keisuke Fukunaga, HUYNH NHAT Kim Phuong, Rumi Shiba, Takayoshi Watanabe

School of Materials Science, Japan Advanced Institute of Science and Technology

P009 Structure and function analysis of the bacterial cell division proteins

#### Hiryoshi Matsumura

College of Life Sciences, Ritsumeikan University

### P010 Crystallographic snapshots of pentameric structure of PBAA, an archaeal homolog of proteasome assembly chaperone

<u>Arunima Sikdar</u><sup>1,2,3</sup>, Tadashi Satoh<sup>3</sup>, Kentaro Kumoi<sup>3</sup>, Kentaro Ishii<sup>2,3</sup>, Maho Yagi-Utsumi<sup>2,3</sup>, and Koichi Kato<sup>1,2,3</sup>

<sup>1</sup>School of Physical Science, SOKENDAI (The Graduate University for Advanced Studies), <sup>2</sup>Okazaki Institute for Integrative Bioscience and Institute for Molecular Science, National Institutes of Natural Sciences, <sup>3</sup>Graduate School of Pharmaceutical Sciences, Nagoya City University

### P011 The first crystal structure of 3.8-MDA supermolecule hemocyanin

<u>Yoshikazu Tanaka</u><sup>1,2,3</sup>, Asuka Matsuno<sup>2</sup>, Zuoqi Gai<sup>1</sup>, Koji Kato<sup>1,2</sup>, Sanae Kato<sup>4</sup>, Takeshi Shimizu<sup>5</sup>, Takeya Yoshioka<sup>5</sup>, Hideki Kishimura<sup>6</sup>, Tohru Terada<sup>7</sup>, Min Yao<sup>1,2</sup>

<sup>1</sup>Faculty of Advanced Life Science, Hokkaido University, <sup>2</sup>Graduate School of Life Science, Hokkaido University, <sup>3</sup>JST, PRESTO, <sup>4</sup>Asahikawa Medical University, 5Hokkaido Industrial Technology Center, <sup>6</sup>Graduate School of Fisheries Science, Hokkaido University, <sup>7</sup>Graduate School of Agricultural and Life Sciences, The University of Tokyo

### P012 Structural basis for dimer formation of human condensin SMC hinge and its binding to DNA

<u>Susumu Uchiyama</u><sup>1,2</sup>, Kazuki Kawahara<sup>3</sup>, Masanori Noda<sup>1</sup>, Takahiro Maruno<sup>1</sup>, Tadayasu Ohkubo<sup>3</sup>, Kiichi Fukui<sup>1</sup>

<sup>1</sup>Graduate School of Engineering, Osaka University, <sup>2</sup>Okazaki Institute for Integrative Bioscience, National Institutes of Natural Sciences, <sup>3</sup>Graduate School of Pharmaceutical Sciences, 3Osaka University

#### P013 Interaction dynamics of DNA and light dependent transcription factor, aureochrome1

<u>Yuki Akiyama</u><sup>1</sup>, Yusuke Nakasone<sup>1</sup>, Osamu Hisatomi<sup>2</sup>, Yoichi Nakatani<sup>2</sup>, Masahide Terazima<sup>1</sup> <sup>1</sup>Graduate School of Science, Kyoto University, <sup>2</sup>Graduate School of Science, Osaka University

### P014 Studies on molecular mechanism of dynamic ordering and disassembling of biomolecular systems

#### Masahide Terazima

Department of Chemistry, Graduate School of Science, Kyoto University

### P015 **Reaction dynamics of light dependent DNA-binding protein EL222** <u>Akira Takakado</u>, Yusuke Nakasone, Masahide Terazima

Graduate School of Science, Kyoto University

#### P016 Creation of dynamic ordering system by artificial light-responsive DNA

Yukiko Kamiya<sup>1,2</sup>, Hideaki Ooi<sup>1</sup>, Hiroyuki Asanuma<sup>1</sup>

<sup>1</sup>Graduate School of Engineering, Nagoya University, <sup>2</sup>Institute of Materials and Systems for Sustainability (IMaSS), Nagoya University

#### P017 Development of fret probe for investigation of the fate of small RNA

<u>Hiroshi Kamimoto</u><sup>1</sup>, Yukiko Kamiya<sup>1,2</sup>, Hiroyuki Asanuma<sup>1</sup> <sup>1</sup>Department of Engineering, Nagoya University <sup>2</sup>Institute of Materials and Systems for sustainability (IMaSS), Nagoya University

### P018 A tightly hybridizable, DNA-like archtecture as a sequence-selective assembly in water Junya Chiba, Masahiko Inouye Graduate School of Pharmaceutical Sciences, University of Toyama

### P019 Heat-induced conformational transition of single-stranded ribonucleic acids: a molecular dynamics simulation study

<u>Yoshiharu Mori</u><sup>1</sup> and Hisashi Okumura<sup>1,2</sup> <sup>1</sup>Institute for Molecular Science, <sup>2</sup>The Graduate University for Advanced Studies

 P020 Development of fluorescence monitoring method for histone deacetylase activity Masafumi Minoshima<sup>1,2</sup>, Yuka Tatematsu<sup>1,2</sup>, <u>Kazuya Kikuchi<sup>1,2</sup></u>
 <sup>1</sup>Graduate School of Engineering, Osaka University, <sup>2</sup>Immunology Frontier Research Center, Osaka Universityy

#### P021 Fluctuating genome structure and gene regulation

M. Sasai, N. Tokuda, S. Fujishiro

Department of Computational Science and Engineering, Nagoya University

#### P022 Structural and functional characterization of HSP27 from CHO cell

<u>Masafumi Yohda</u><sup>1</sup>, Eiryo Sha<sup>1</sup>, Yohei Y. Yamamoto<sup>1</sup>, Toshihiko Oka<sup>2</sup>, Keiichi Noguchi<sup>3</sup> <sup>1</sup>Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology, <sup>2</sup>Department of Physics, Shizuoka University, <sup>3</sup>Instrumentation Analysis Center, Tokyo University of Agriculture and Technology

### P023 Disassembly of the self-assembled, double-ring structure of proteasome α7 homo-tetradecamer by α6

<u>Kentaro Ishii</u><sup>1</sup>, Masanori Noda<sup>2</sup>, Hirokazu Yagi<sup>3</sup>, Ratsupa Thammaporn<sup>4</sup>, Supaporn Seetaha<sup>4</sup>, Tadashi Satoh<sup>3</sup>, Koichi Kato<sup>1,3,5</sup>, Susumu Uchiyama<sup>1,2</sup>

<sup>1</sup>Okazaki Institute for Integrative Bioscience, <sup>2</sup>Graduate School of Engineering, Osaka University, <sup>3</sup>Graduate School of Pharmaceutical Sciences, Nagoya City University, <sup>4</sup>Faculty of Science, Kasetsart University, <sup>5</sup>Institute for Molecular Science

### P024 Dynamical feature of huge aggregated protein, α B-crystallin

<u>Masaaki Sugiyama</u><sup>1</sup>, Rintaro Inoue<sup>1</sup>, Noriko Fujii<sup>1</sup>, Kentaro Ishii<sup>2</sup>, Susumu Uchiyama<sup>2,3</sup> <sup>1</sup>Research Reactor Institute, Kyoto University, <sup>2</sup>Okazaki Institute for Integrative Bioscience, <sup>3</sup>Graduate School of Engineering, Osaka University

#### P025 The effect of the structural compressibility change on the reaction of SyPixD

<u>Tsubasa Nakajima</u><sup>1</sup>, Kunisato Kuroi<sup>2</sup>, Kouji Okajima<sup>3,4</sup>, Masahiko Ikeuchi<sup>4</sup>, Satoru Tokutomi<sup>3</sup>, Masahide Terazima<sup>1</sup>,

<sup>1</sup>Graduate School of Science, Kyoto University, <sup>2</sup>Institute for Molecular Science, <sup>3</sup>Graduate School of Science, Osaka Prefecture University, <sup>4</sup>Graduate School of Arts and Science, Tokyo University

### P026 Exploring regulatory association and dissociation processes of biological molecules constituting a functional module

#### Hironari Kamikubo

Graduate School of Materials Science, Nara Institute of Science and Technology

### P027 Structural investigation of direct interaction between Shootin1 and cortactin by the titration SAXS measurements

Junko Makino<sup>1</sup>, Keito Yoshida<sup>1</sup>, Yusuke Kubo<sup>2</sup>, Kentarou Baba<sup>2</sup>, Yoichi Yamazaki<sup>1</sup>, Naoyuki Inagaki<sup>2</sup>, Mikio Kataoka<sup>1</sup>, Hironari Kamikubo<sup>1</sup>

<sup>1</sup>Graduate School of Materials Science, Nara Institute of Science and Technology <sup>2</sup>Graduate School of Biological Sciences, Nara Institute of Science and Technology

### P028 Functional analysis of a splicing isoform of shootin1

Takunori Minegishi, Wataru Yoshida, Yasuyuki Uesugi, <u>Naoyuki Inagaki</u> Graduate School of Biological Sciences, Nara Institute of Science and Technology

### P029 SAXS study on early aggregation preceding the nucleation of insulin amyloid fibrils

<u>Eri Chatani</u><sup>1</sup>, Rintaro Inoue<sup>2</sup>, Hiroshi Imamura<sup>3</sup>, Masaaki Sugiyama<sup>2</sup>, Minoru Kato<sup>3</sup>, Masahide Yamamoto<sup>4</sup>, Koji Nishida<sup>5</sup>, Toshiji Kanaya<sup>5</sup>

<sup>1</sup>Graduate School of Science, Kobe University, <sup>2</sup>Research Reactor Institute, Kyoto University, <sup>3</sup>College of Pharmaceutical Science, Ritsumeikan University, <sup>4</sup>Kyoto University, <sup>5</sup>Institute for Chemical Research, Kyoto University

### P030 Elucidating the mechanisms of the amyloid fibril formation via prefibrillar intermediates; a case study on insulin b chain

<u>Naoki Yamamoto</u><sup>1</sup>, Shoko Tsuhara<sup>1</sup>, Eri Chatani<sup>1</sup> <sup>1</sup>Graduate School of Science, Kobe University

### P031 Regulation of amyloid formation by targeting the conformational fluctuations of immunoglobulin light chain variable domain

Daizo Hamada<sup>1,2,3</sup>

<sup>1</sup>Graduate School of Medicine and <sup>2</sup>Graduate School of Engineering, Kobe University, <sup>3</sup>Community-University Research Cooperation Center, Mie University

### P032 Fibril inhibition mechanism of human calcitonin by curcumin as revealed by NMR and MD simulation

Hikari Itoh-Watanabe<sup>1</sup>, Ken Takeuchi<sup>1</sup>, Kengo Daidoji<sup>1</sup>, Shuhei Toyoda<sup>1</sup>, Namsrai Javkhalantugs<sup>1,2</sup>, Izuru Kawamura<sup>1</sup>, Kazuyoshi Ueda<sup>1</sup>, Hiroshi Hirota<sup>3</sup>, Tsutomu Nakayama<sup>4</sup>, <u>Akira Naito<sup>1</sup></u>

<sup>1</sup>Graduate School of Engineering, Yokohama National University, <sup>2</sup>Center for Nanoscience and Nanotechnology, School of Engineering, School of Engineering and Applied Science, National

University of Mongolia, <sup>3</sup>Antibiotic Laboratory, Riken, <sup>4</sup>Nippon Verterinary and Life Science University

#### P033 Analysis of amyloid formation and inhibition mechanisms of human calcitonin

<sup>1</sup><u>Chiaki Ota</u>, <sup>1</sup>Hiroko Tanaka, <sup>2</sup>Tomoyasu Aizawa, <sup>1</sup>Yoichi Yamazaki, <sup>1</sup>Mikio Kataoka, <sup>1</sup>Hironari Kamikubo

<sup>1</sup>Grad. Sch. Mat. Sci., NAIST, <sup>2</sup>Graduate School of Life Science, Hokkaido University

#### P034 All-atom molecular dynamics simulations of Aβ amyloid fibril

Hisashi Okumura<sup>1,2</sup>, Satoru G. Itoh<sup>1,2</sup>

<sup>1</sup>Research Center for Computational Science, Institute for Molecular Science, <sup>2</sup>Department of Structural Molecular Science, The Graduate University for Advanced Studies

#### P035 Transient dimerization and conformational changes of blue light sensor protein phototropin

<u>Yusuke Nakasone</u><sup>1</sup>; Koji Okajima<sup>2</sup>; Yusuke Aihara<sup>1</sup>; Akira Nagatani<sup>1</sup>; Satoru Tokutomi<sup>2</sup>; Masahide Terazima<sup>1</sup>

<sup>1</sup>Graduate School of Science, Kyoto University, <sup>2</sup>Graduate School of Science, Osaka Prefecture University.

### P036 Dynamic structural change of Blrp1 detected by transient grating method

Kosei Shibata, Yusuke Nakasone, Masahide Terazima Graduate School of Science, Kyoto University

### P037 Signaling kinetics of cyanobacterial phytochrome (Cph1)

<u>Kimitoshi Takeda</u>, Masahide Terazima Department of Chemistry, Kyoto University

P038 H-bonding geometry of photoactive yellow protein calculated by combination of oniom and multicomponent quantum mechanics

Yusuke Kanematsu and <u>Masanori Tachikawa</u> Graduate School of NanoBioScience, Yokohama City University

### P039 Dynamic interaction between Kai proteins dependent on phosphorylation states of KaiC revealed by HS-AFM

<u>Takayuki Uchihashi</u><sup>1</sup>, Tetsuya Mori<sup>2</sup>, Shogo Sugiayma<sup>1</sup>, Carl H. Johnson<sup>2</sup>, Toshio Ando<sup>1</sup> <sup>1</sup>Department of Physics/Bio-AFM FRC, Kanazawa University, <sup>2</sup>Department of Biological Sciences, Vanderbilt University

- P040 Studies on cyanobacterial circadian clock system from different perspectives
   Jun Abe<sup>1</sup>, Atsushi Mukaiyama<sup>1,2</sup>, Yoshihiko Furuike<sup>1,2</sup>, <u>Shuji Akiyama<sup>1,2</sup></u>
   <sup>1</sup>Institute for Molecular Science, <sup>2</sup>SOKENDAI
- P041 Insight into the function of alanine-422 residue of KaiC involved in resetting of the cyanobacterial circadian clock Kazuki Nagata<sup>1</sup>, <u>Kazuki Terauchi<sup>1, 2</sup></u> <sup>1</sup>Graduate School of Life Sciences, <sup>2</sup>Department of Life Sciences, Ritsumeikan University
- P042 Punctuation mechanism of artificial protein needle <u>Takafumi Ueno<sup>1</sup></u>, Takayuki Uchihashi<sup>2</sup>, Tadaomi Furuta<sup>1</sup>
   <sup>1</sup>Department of Bioscience and Biotechnology, Tokyo Institute of Technology, <sup>2</sup>Department of Physics, Kakazawa University

### P043 Complete and peptide-bound structures of the Sec translocon

<u>Yoshiki Tanaka</u><sup>1</sup>, Yasunori Sugano<sup>1</sup>, Mizuki Takemoto<sup>2,3</sup>, Takaharu Mori<sup>4</sup>, Arata Furukawa<sup>1</sup>, Tsukasa Kusakizako<sup>2,3</sup>, Kaoru Kumazaki<sup>2,3</sup>, Ayako Kashima<sup>1</sup>, Ryuichiro Ishitani<sup>2,3</sup>, Yuji Sugita<sup>4</sup>, Osamu Nurek<sup>i2,3</sup>, Tomoya Tsukazaki<sup>1,5</sup>

<sup>1</sup>Department of Systems Biology, Nara Institute of Science and Technology, <sup>2</sup>Department of Biological Sciences, The University of Tokyo, <sup>3</sup>Global Research Cluster, RIKEN, <sup>4</sup>Theoretical Molecular Science Laboratory, RIKEN, <sup>5</sup>JST, PRESTO

P044 Restless crowds of the KcsA potassium channels inside a cluster: high speed AFM imaging and effects of the membrane lipids
 Ayumi Sumino<sup>1</sup>, Takayuki Uchihashi<sup>2</sup>, Shigetoshi Oiki<sup>1</sup>

<sup>1</sup>Faculty of Medical Sciences, University of Fukui, <sup>2</sup>Graduate School of Science, Kanazawa University

P045 Alteration of lipid packing states by curvature inducing peptides to promote membrane translocation of arginine-rich cell-penetrating peptides

Shiroh Futaki, Tomo Murayama

Institute for Chemical Research, Kyoto University

### P046 Visualization of COPII minimal machinery during membrane association in an artificial planar lipid bilayer

<u>Hirohiko Iwasaki, Ken Sato</u> Depatment of Life Sciences, Graduate School of Arts and Sciences, University of Tokyo

### P047 Catalyst-producing system in a self-reproducing giant vesicle

Kensuke Kurihara<sup>1,2,3</sup>, Li Sheng<sup>1,2</sup>

<sup>1</sup>Deptartment of Bioorganization Research, Okazaki Institute for Integrative Bioscience, <sup>2</sup>Institute for Molecular Science, <sup>3</sup>Research Center for Complex Systems Biology, The University of Tokyo

### P048 Energy transfer process in DPPC/cholesterol lipid bilayer membrane observed with picosecond time-resolved Raman spectroscopy

Sho Kitamura, Tomohisa Takaya, <u>Koichi Iwata</u> Department of Chemistry, Gakushuin University

P049 Impact of local anethetics on the SM-rich domain formed in artificial raft membranes Masanao Kinoshita, Takeshi Chitose, Nobuaki Matsumori Department of Chemistry, Faculty of Science, Kyushu University

## P050 Integrrated analysis of lipid rafts <u>Nobuaki Matsumori</u><sup>1</sup>, Masanao Kinoshita<sup>1</sup>, Michio Murata<sup>2,3</sup> <sup>1</sup>Department of Chemistry, Kyushu University, <sup>2</sup>Department of Chemistry, Osaka University, <sup>3</sup>JST-ERATO

P051 Screening of the agents to overcome drug resistance of human hepatoma HEPG2 cells by using

three-dimensional culture

<u>Takahiro Mizutami</u>, Yuya Ohta, Yuji Komizu, Taku Matsushita Dept. of Applied Life Science, Sojo University

### P052 Mechanical activity of dynein and its dynamical ordering underlying oscillatory movement of sperm flagella

Chikako Shingyoji<sup>1</sup>, Hiroshi Yoke<sup>1</sup>, Izumi Nakano<sup>1</sup>, Yuichi Inoue<sup>2</sup>, Hideo Higuchi<sup>3</sup>

<sup>1</sup>Department of Biological Sciences, Graduate School of Science, The University of Tokyo, <sup>2</sup>Institute of Multidisciplinary Research, Tohoku University, <sup>3</sup>Department of Physics, Graduate School of Science, The University of Tokyo

 P053
 Formation of bioinspired π-system-ion complexes exhibiting dynamic ordering

 Hiromitsu Maeda

College of Pharmaceutical Sciences, Ritsumeikan University

- P054 Simple conformational search algorithms for folding problems
   <u>Yasuteru Shigeta</u> and Ryuhei Harada
   Department of Physics, Graduate School of Pure and Applied Sciences, University of Tsukuba
- P055 Oligomer formation pathway of Aβ fragments by coulomb replica-permutation MD simulations Satoru G. Itoh<sup>1,2</sup>, Hisashi Okumura<sup>1,2</sup>
   <sup>1</sup>Institute for Molecular Science, <sup>2</sup>The Graduate University for Advanced Studies
- P056 replica-exchange molecular dyamics simulation of n-glycans in Fc complexed with FcγRIIIa
   <u>Yoshitake Sakae</u><sup>1</sup>, Takumi Yamaguchi<sup>2</sup>, Tadashi Sato<sup>3</sup>, Saeko Yanaka<sup>2</sup>, Koichi Kato<sup>2</sup>, Yuko Okamoto<sup>1</sup>
   <sup>1</sup>Department of Physics, Nagoya University, <sup>2</sup>Institute for Molecular Science, <sup>3</sup>Department of Structural Biology and Biomolecular Engineering, Nagoya City University
- P057 Dependence of effective interaction between macroanions in electrolyte solution on valence of co-ions

Takumi Yamashita, Ryo Akiyama Department of Chemistry, Kyushu University

- P058 Aggregation of acidic proteins and effective attraction between like-charged particles <u>Takuto Sawayama</u>, Ryo Akiyama Department of Chemistry, Kyushu University
- P059 Effects of depletion interaction on the crystallization
   <u>Ayumi Suematsu</u><sup>1</sup>, Akira Yoshimori<sup>1,2</sup>,, Ryo Akiyama<sup>1</sup>
   <sup>1</sup>Depertment of Physics, Kyushu University, <sup>2</sup>Depertment of Physics, Niigata University

### P060 Distinct dissociation kinetics between ion pairs: solvent-coordinate free-energy landscape analysis

#### Yoshiteru Yonetani

Quantum Beam Science Center, Japan Atomic Energy Agency

P061 Theoretical study on a pyrrole rotation of the anion binding system with DFT calculation
 <u>Tomoki Kato</u>, Yui Sakuma, Takako Mashiko, Masanori Tachikawa
 Division of Materials Science, International College of Arts and Sciences, Yokohama City University

# P062 Exploration of the structure of the folding intermediate by MD simulations <u>Yukihito Kajikawa</u><sup>1</sup>, Yuko Okamoto<sup>1,2,3,4</sup> <sup>1</sup>Grad. Sch. Sci., Nagoya Univ., <sup>2</sup>Struct. Biol. Res. Center, Grad. Sch. Sci. Nagoya Univ., <sup>3</sup>Center Comput. Sci., Grad. Sch. Eng., Nagoya Univ., <sup>4</sup>Info. Tech. Center, Nagoya Univ.

### P063 Master equation analysis on intermediates in self assembly process of an octahedron-shaped coordination capsule

Y. Matsumura<sup>1</sup>, S. Hiraoka<sup>2</sup>, H. Sato<sup>1,3</sup>

<sup>1</sup>Department of Molecular Engineering, Kyoto University, <sup>2</sup>Department of Basic Science, Graduate School of Arts and Sciences, The University of Tokyo, <sup>3</sup>ESICB, Kyoto University

### P064 **Predicting epitope of omalizumab to IgE using MD simulations**

Hiroyuki Kawamoto<sup>1</sup>, Yuko Okamoto<sup>1,2,3,4</sup>

<sup>1</sup>Grad. Sch. Sci., Nagoya Univ.; <sup>2</sup>Struc. Biol. Res. Center, Grad. Sch. Sci. Nagoya Univ.; <sup>3</sup>Center Comp. Sci., Grad. Sch. Eng., Nagoya Univ., Info. <sup>4</sup>Tech. Center, Nagoya Univ

### P065 Role of calcium ion in molecular recognition process of calcium-dependent carbohydratebinding module

S. Tanimoto<sup>1</sup>, N. Yoshida<sup>1</sup>, M. Higashi<sup>2</sup>, and H. Nakano<sup>1</sup>

<sup>1</sup>Department of Chemistry, Graduate School of Sciences, Kyushu University, <sup>2</sup>Department of Chemistry, Biology and Marine Science, University of the Ryukyu

#### P066 Role of water on domain-swapped oligomer formation of Cytochrome C

Norio Yoshida<sup>1</sup>, Masahiro Higashi<sup>2</sup>, Shun Hirota<sup>3</sup>

<sup>1</sup>Department of Chemistry, Graduate School of Science, Kyushu University, <sup>2</sup>Department of Chemistry,

Biology and Marine Science, University of the Ryukyus, <sup>3</sup>Graduate School of Materials Science, Nara Institute of Science and Technology

### P067 Replica-exchange molecular dynamics simulations of metal-ligand self-assembly into nanosphere ML

<u>Yuhei Tachi<sup>1</sup></u>, Sota Sato<sup>2</sup>, Makoto Yoneya<sup>3</sup>, Yuko Okamoto<sup>1</sup>

<sup>1</sup>Department of Physics, School of Science, The University of Nagoya, <sup>2</sup>WPI-AIMR, and Department of Chemistry, School of Science, The University of Tohoku, <sup>3</sup>Nanosystem Research Institute, National Institute of Advanced Industrial Science and Technology

### P068 Interactions among biological molecular assembly and among artificial molecular assembly and large-scale structural transformations

Yuko Okamoto<sup>1,2,3,4,5</sup>

<sup>1</sup>Dept. Physics, Grad. Sch. Sci., Nagoya Univ., <sup>2</sup>Struct. Biol. Res. Center, Grad. Sch. Sci., Nagoya Univ., <sup>3</sup>Center Comput. Sci., Grad. Sch. Eng., Nagoya Univ., <sup>4</sup>Info. Tech. Center, Nagoya Univ., <sup>5</sup>JST-CREST

#### P069 Estimating structural stability of self-assembled clusters

Yuichiro Yoshida<sup>1</sup> and Hirofumi Sato<sup>1,2</sup>

<sup>1</sup>Graduate School of Engineering, Kyoto University, <sup>2</sup>Elements Strategy Initiative for Catalysts and Batteries, Kyoto University

### P070 Molecular theories for self-organization and order formation

Hirofumi Sato<sup>1,2</sup>, Takeshi Yamamoto<sup>3</sup>

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### P071 The effect of substituted groups on the stability of nanocube consisting of gear-shaped amphiphiles

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P072 **Optoelectronic properties of self-assembled molecular systems** Takatoshi Fujita, Takeshi Yamamoto Department of Chemistry, Graduate School of Science, Kyoto University

P073 Theoretical study with the CH3 groups of self-assembled nanocube in aqueous methanol solvent <u>Takako Mashiko<sup>1</sup></u>, Shuichi Hiraoka<sup>2</sup>, Umpei Nagashima<sup>3</sup>, Masanori Tachikawa<sup>1</sup>
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P074 Self assembly of gear-shaped amphiphiles into a molecular capsule (nanocube): computational study

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P075 Final stage of the self-assembly process on [Pd<sub>2</sub>L<sub>4</sub>]<sub>4</sub>+cage complex in solvent with DFT calculation

<u>Yui Sakuma</u><sup>1</sup>, Takako Mashiko<sup>1</sup>, Shuichi Hiraoka<sup>2</sup>, Umpei Nagashima<sup>3</sup>, Masanori Tachikawa<sup>1</sup> <sup>1</sup>Graduate School of Nanobioscience, Yokohama City University, <sup>2</sup>Graduate School of Arts and Sciences, The University of Tokyo, <sup>3</sup>FOCUS

### P076 Self-assembly process of coordination assemblies and development of supramolecular cube with extremely high thermal stability

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### P077 The importance of triple-π interaction and Van der Waals interaction for the thermal stability of nanocube based on gear-shaped amphiphiles

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### P078 Dynamic chirality transfer from structurally switchable helical metal complex for regulating supramolecular helicity

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#### P079 Self-assembly process of coordination macrocycles

<u>Ayako Baba</u>, Tatsuo Kojima, Shuichi Hiraoka Graduate School of Arts and Sciences, The University of Tokyo

### P080 Relaxation phenomena and development of structure in a physically cross-linked telechelic polymers

<u>Masahiko Annaka</u>, Shintaro Yashima Graduate School of Science, Kyushu University

### P081 The self-assembly process of Pd<sub>2</sub>L<sub>4</sub> coordination cages

<u>Shumpei Kai</u>, Tatsuo Kojima, Shuichi Hiraoka Graduate School of Arts and Sciences, University of Tokyo

 P082
 Development of dynamical ordering of artificial molecules by mimicking biomolecular systems

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### P083 Accommodation of steroids within a synthetic cavity

<u>Taito Kato</u>, Tomohisa Sawada, Makoto Fujita Graduate School of Engineering, The University of Tokyo

- P084 Artificial peptide-based nanostructures via coordination-driven folding and assembly <u>Tomohisa Sawada</u>, Motoya Yamagami, Yusuke Otsubo, Asami Matsumoto, Makoto Fujita Graduate School of Engineering, The University of Tokyo
- P085 Specific recognition of d-amino-acid-containing short peptides by a synthetic cavity <u>Kiyohiro Adachi</u>, Tomohisa Sawada, Makoto Fujita Graduate School of Engineering, The University of Tokyo
- P086 Synthesis of macromolecular [2]rotaxane having poly(ethylene oxide) as an axle component and its application to rotaxane cross-linked polymers

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## P087Functionalization of a self-assembled tetrahedral capsuleMasatoshi Mori, Tomohisa Sawada, Makoto FujitaGraduate School of Engineering, The University of Tokyo

## P088 Synthesis and dynamical assembly of polymers connected by rotaxane linkage Daisuke Aoki, <u>Toshikazu Takata</u> Department of Organic and Polymeric Materials, Tokyo Institute of Science and Technology

# P089 Phase separation of thermosensitive polymers induced by chemical reaction <u>Masami Naya</u><sup>1</sup>, Yoshiki Kuroshima<sup>2</sup>, Yoshimi Hamano<sup>1</sup>, Kenta Kokado<sup>1,2,3</sup>, Kazuki Sada<sup>1,2,3</sup> <sup>1</sup>Graduate School of Chemical Sciences and Engineering, Hokkaido University, <sup>2</sup>Department of Chemistry, School of Science, Hokkaido University, <sup>3</sup>Department of Chemistry, Faculty of Science, Hokkaido University

### P090 Construction of metal-organic frameworks (MOF) -motor protein conjugates

Masaki Ito<sup>1</sup>, Takumi Ishiwata<sup>1</sup>, Kenta Kokado<sup>1,2</sup>, Akira Kakugo<sup>1,2</sup>, <u>Kazuki Sada<sup>1,2</sup></u> <sup>1</sup>Graduate School of Chemical Sciences and Engineering, & <sup>2</sup>Faculty of Science, Hokkaido University

### P091 Synthesis and properties of hydrogel particles prepared with cyclodextrin type pseudopolyrotaxane cross-linkers

<u>Daichi Aoki</u><sup>1</sup>, Seina Hiroshige<sup>1</sup>, Takuma Kureha<sup>1</sup>, Keisuke Iijima<sup>3</sup>, Daisuke Aoki<sup>3</sup>, Toshikazu Takata<sup>3</sup>, Daisuke Suzuki<sup>1,2</sup>

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### P092 Control of oscillation period of smart polymer hydrogel particles driven by chemical reaction Shusuke Matsui<sup>1</sup>, Yuki Sakurai<sup>1</sup>, <u>Daisuke Suzuki</u><sup>1,2</sup> <sup>1</sup>Graduate School of Textile Science & Technology, Shinshu University, <sup>2</sup>Division of Smart Textiles, Institute for Fiber Engineering, Interdisciplinary Cluster for Cutting Edge Research, Shinshu University

### P093 Microscopic structural changes in hydrogel particles in the presence of target molecules

#### investigated by small- and wide-angle X-ray scattering

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### P094 Membrane curvature controls the dynamics of COPII coat during vesicle formation

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